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A NEW ELECTRONIC TRANSITION IN SeO

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ABSTRACT

A new electronic band-system in emission has been recorded in the region $6150-5250 \text{ \AA}^0$ using a transformer discharge through flowing SeO_2 vapor. Twentyfour weak red degraded bands have been observed and are attributed to the molecule SeO . A vibrational analysis of the observed bands leads to the conclusion that the upper state involved in the transition is new state b which is situated at 17338.5 cm^{-1} above the ground state. The lower state involved in the transition is the ground state of the molecule. The values of ω_e and $\omega_{e\pi}$ for the upper and lower states are found to be :

$$\begin{aligned} \text{Upper State b : } \omega_e &= 885.2 \text{ cm}^{-1}, & \omega_{e\pi} &= 5.85 \text{ cm}^{-1} \\ \text{Lower State X : } \omega_e &= 914.8 \text{ cm}^{-1}, & \omega_{e\pi} &= 4.87 \text{ cm}^{-1} \end{aligned}$$

INTRODUCTION

The electronic band-system of SeO has been investigated by Asundi et al (1), Choong (2), and Barrow et al (3). Only one band-system involving the ground state X and the upper state A has been known so far. According to the work of Barrow et al (3) the upper and the lower states involved in the transition $A \rightarrow X$ are both $3 \Sigma^-$.

A literature survey of the electronic band-system of the monoxides of group VIA elements reveals that in TeO, O₂ and SO more than one electronic band-system has been known. In the molecule NBr (4) which is isoelectronic with SeO, a band-system has been known in the region 6400-5650 Å°. The present investigation was undertaken with a view to discover new electronic transitions in SeO, and a new band-system in the region (6150-5250 Å°) has been recorded in addition to the known A - X system. From our studies we have concluded that this new electronic transition involve the ground state X and a new upper electronic state which we have labeled as the b-state.

EXPERIMENTAL

The emission spectrum of SeO was recorded by exciting a pure sample of SeO₂ under flowing condition in a conventional K - type discharge tube using a power transformer. The chemical was 99.9% pure and was obtained from May and Backer Ltd., London. The band-spectra were recorded on Ilford-HP3 hyper sensitive panchromatic plates on a Steinheil 3-prism glass spectrograph which has a reciprocal linear dispersion of about 3Å°/mm. at 4400 Å°. The exposure time and slit width were 3-hours and 20 microns respectively. The intensity of the recorded bands was found to be very weak (too weak to be reproduced in a journal). The observed bands were measured on a Russian made Comparator (Model No. EZA-2) using iron lines as reference. The band heads of the more intense bands were measured with a precision of $\pm 2 \text{ cm}^{-1}$. The weaker bands were measured with a precision of $\pm 4 \text{ cm}^{-1}$ by making pinholes at the position of their band heads.

RESULTS AND DISCUSSIONA : The known A-X system:

Excitation of the SeO_2 in the discharge tube gave rise to the known A-X system of SeO. Ten strong bands of this system were measured and their wavelengths were found to agree with those reported by Pearse and Gaydon (5).

B: The New Band-System :

Twentyfour weak bands, degraded to the red were observed in the region 6150-5130 \AA^0 . The wavelength, wavenumber, and the vibrational assignment of the bands are entered in Table I. The bands fit very nicely into the Deslandres' scheme of a diatomic molecule as shown in Table II. The molecular constants obtained from the vibrational analysis have been entered in Table III.

The value of the ω_e for the lower state has been found to be 914.8 cm^{-1} which agrees very well with the ground state frequency of 914.69 cm^{-1} reported by Barrow et al (3), giving a very strong evidence that the lower state involved in the transition of this new system is the $X^3\Sigma^-$ state of SeO.

The value of ω_e for the upper state has been found to be 895.2 cm^{-1} . On the basis of our experimental data it is not possible to arrive at any conclusion regarding the nature of this upper electronic state of the molecule which we have labeled as b-state. However, we observe that in O_2 (6) and in SO (7) a low-lying $b^1\Sigma^+$ state has been found ^{and} a forbidden transition $b^1\Sigma^+ - X^3\Sigma^-$ has also been observed. The values of ω_e , ω_e' and the ratio ω_e/ω_e'' for the $b^1\Sigma^+$ and $X^3\Sigma^-$ states in O_2 and SO have been given in Table IV, and

TABLE I
 Wavelengths, Wavenumbers, and the Vibrational
 Assignment of the New Bands of SeO

S.No.	Wavelengths in Å	Wavenumbers (vacuum) in cm^{-1}	Assignment (ν' , ν'')
1	6139.1	16284	(6,7)
2	6117.3	16343	(4,5)
3	6106.6	16371	(3,4)
4	6095.4	16401	(2,3)
5	6088.3	16420	(1,2)
6	6079.5	16444	(0,1)
7	5835.9	17130	(6,6)
8	5821.7	17172	(5,5)
9	5809.5	17208	(4,4)
10	5796.1	17248	(3,3)
11	5784.0	17284	(2,2)
12	5773.0	17317	(1,1)
13	5762.4	17349	(0,0)
14	5574.7	17933	(7,6)
15	5558.6	17985	(6,5)
16	5543.1	18035	(5,4)
17	5528.8	18062	(4,3)
18	5513.2	18133	(3,2)
19	5499.8	18177	(2,1)
20	5486.0	18223	(1,0)
21	5287.8	18906	(5,3)
22	5271.3	18965	(4,2)
23	5254.2	19027	(3,1)
24	5239.3	19081	(2,0)

TABLE II

Deslandres' Scheme for the New Bands of SeO

v''	0	1	2	3	4	5	6	7
v'								
0	17349 905 16444							
	874	873						
1	18223 906 17317 897 16420							
	858	860	864					
2	19061 904 18177 893 17284 883 16401							
	850	849	847					
3	19027 894 18133 885 17248 877 16371							
	832	834	837					
4	18965 883 18082 874 17208 865 16343							
	824	827	829					
5	18906 871 18035 863 17172							
			813					
6				17985 855 17130 846 16284				
				803				
7					17933			

we find that the molecule SeO fits into the trend nicely. This observation together with the fact that the intensity of the bands of this new system is quite weak leads to the suggestion that the transition involved is probably $b^1\Sigma^+ - X^3\Sigma^-$. Of course, the rotational structure of the bands must be resolved and studied before arriving at any definite conclusion regarding the nature of the upper electronic state.

TABLE III

Molecular Constants for the b and X States of SeO

State	ω_e (cm ⁻¹)	ω_e (cm ⁻¹)	ω_a (cm ⁻¹)
b	17338.5	885.2	5.8 ₅
X	0	914.8	4.8 ₇

TABLE IV

 ω_e and ω_a and ω_e/ω_a in the b and X States of O₂, SO and SeO

Molecule	ω_e (cm ⁻¹)	ω_a (cm ⁻¹)	$\frac{\omega_e}{\omega_a}$	Ref.	Electronic Transition	Wavelength region A
O ₂	1432.68	1580.36	0.91	6	b $^1\Sigma^+$ - X $^3\Sigma^-$	(5380-8803)
SO	1068.66	1149.22	0.94	7	b $^1\Sigma^+$ - X $^3\Sigma^-$	(9600-10500)
SeO	885.2	914.8	0.95	Presnt work	b $^1\Sigma$ - X $^3\Sigma^-$	(5250-6150)

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